PRELIMINARY MODEL-COMPARISON RESULTS FROM THE SIM-SEQ PROJECT USING TOUGH2, STOMP, ECLIPSE, AND VESA APPROACH

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ABSTRACT

Sim-SEQ is an international initiative on model comparison for geologic carbon sequestration (GCS), with an objective to understand and, if possible, quantify model uncertainties. Model comparison efforts in Sim-SEQ are initially limited to one specific field test site, hereafter referred to as the Sim-SEQ Study site (or S-3 site). Within Sim-SEQ, different modeling teams are developing conceptual models of CO_2 injection at the S-3 site. One of the conceptual models, developed by the LBNL team, is based on TOUGH2/EOS7C. In this paper, we present some preliminary model predictions of the S-3 site using the TOUGH2/EOS7C simulator. We also compare the predictions of the TOUGH2 simulator with three other conceptual models, developed by three different organizations, of the S-3 site.

INTRODUCTION

Because of the complexities of subsurface flow and transport processes, choices made while developing conceptual and numerical models for GCS applications may result in a wide range of model predictions, even with each of these models considering the same injection scenario at the same GCS site.

To identify the sources of model uncertainty and, if possible, quantify these uncertainties, we must perform a model comparison study involving both model-to-data and model-to-model comparisons at one or more selected GCS field sites. To accomplish this goal, the United States Department of Energy (USDOE) has initiated a model comparison study, named Sim-SEQ, for GCS.

The objectives of Sim-SEQ, its scope, and its present status can be found in Mukhopadhyay et al. (2012). Briefly, the Sim-SEQ project intends to objectively evaluate the modeling efforts of different groups as they are applied to CO_2 injection field tests. Sim-SEQ began in April 2011 with four modeling teams (all from the United States), but has since then rapidly developed into an international collaboration project with 15 modeling teams from eight countries. A list of the organizations/institutes participating in Sim-SEQ, and the software/modeling approaches that these teams are using, is provided in Mukhopadhyay et al. (2012).

The primary focus of the model comparison effort in the Sim-SEQ project is to correctly predict the behavior of the injected CO_2 plume at the S-3 site. The target formation for injection at the S-3 site comprises fluvial deposits of considerable heterogeneity and is located in the water leg of an active CO_2-EOR field with a strong water drive (Hovorka et al., 2011). These features add significant complexity when approximating the natural system, and challenges arise in dealing with boundary conditions. In addition, the presence of methane has been confirmed in the brine, which can potentially exsolve and impact pressure buildup history and CO_2 plume extent.

The TOUGH2 numerical code (Pruess et al., 1999) has an established reputation for reliably simulating flow and transport behavior in complex subsurface systems. The first objective of this paper is to present a conceptual model of the CO_2 injection scenario at the S-3 site based on the EOS7C module (Oldenburg et al., 2004) of the TOUGH2 simulator, and to illustrate its usefulness in simulating a complex geological system comprised of water, supercritical CO_2, and CH_4. Our second objective is to compare the TOUGH2 predictions against results from other conceptual models based on different simulators. For this purpose, we have selected results from three other groups within the Sim-SEQ project.

We begin the paper by briefly introducing the S-3 site. We then describe the conceptual representation of the S-3 site based on TOUGH2 and the other three conceptual models. Next, we present the results based on TOUGH2 and compare them against the other three models. The paper concludes by summarizing the findings from this preliminary model comparison study, and by making recommendations for future extensions of the Sim-SEQ project.

THE S-3 SITE

The S-3 site is patterned after the Southeast Regional Carbon Sequestration Partnership (SECARB) Phase III Early Test in the southwestern part of Mississippi (USA). A description of the geology of the site can be found in Hovorka et al. (2011). The target formation for injection at the S-3 site is comprised of fluvial sandstones of the Cretaceous lower Tuscaloosa Formation at depths of 3300 m, which form a 4-way anticline cut by a northwest-trending fault (Figure 1). The complex geological features of the site present an opportunity for studying how well the sedimentary architecture controls fluid flow.

Denbury Onshore LLC (hereafter referred to as Denbury) has hosted the SECARB Phase II and Phase III tests in a depleted oil and gas reservoir under CO_2 flood since 2007. The tests are managed by the Bureau of Economic Geology (BEG) at the University of Texas, Austin. The Phase III Early Test started in April 2009 with CO_2 injection in the eastern block of the northwest-trending fault, in an area commonly known as the High Volume Injection Test (HiVIT) area, as shown in Figure 1. The Sim-SEQ project focuses on one part of the HiVIT, referred to as the Detailed Area Study (DAS), located in the water leg of the reservoir, outside of but close to the reservoir under CO_2 flood.

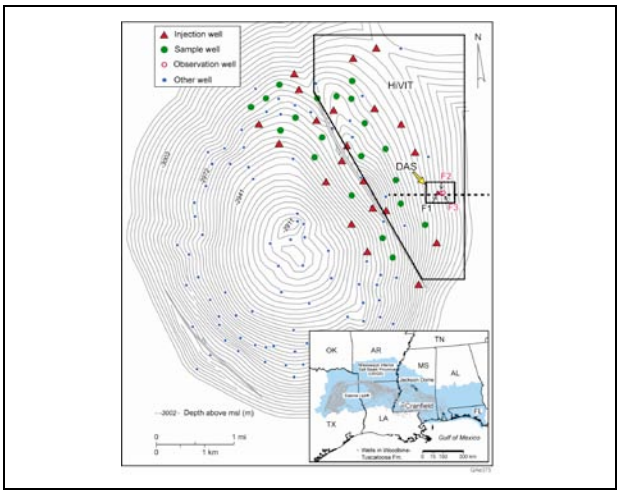

Figure 1. Location map of the S-3 site including the HiVIT and DAS

The DAS area has been designed to collect dense time-lapse data from an array of three closely spaced wells (i.e., F-1, F-2, and F-3), with injection occurring through well F-1 and the other two serving as observation wells, located downdip of F-1. The surface locations of the three wells are aligned approximately in an east-west direction, with F-2 positioned 70 m of F-1 to the west and 30 m of F-3 to the east. Injection in the DAS area (through well F-1) started in December 2009. The observed injection rate and the bottomhole temperature at the injection well are shown in Figure 2.

CONCEPTUAL MODELS

Here, we focus on four different conceptual models of the S-3 site. These models are the LBNL Model (developed by Lawrence Berkeley National Laboratory), the PNNL Model (developed by the Pacific Northwest National Laboratory), the ICL Model (developed by Imperial College, London) and the Vertical Equilibrium Sub-scale Analytical or VESA Model (developed by Center for Integrated Petroleum Research, Uni Research, Norway). We first present the essential features of these four conceptual models.

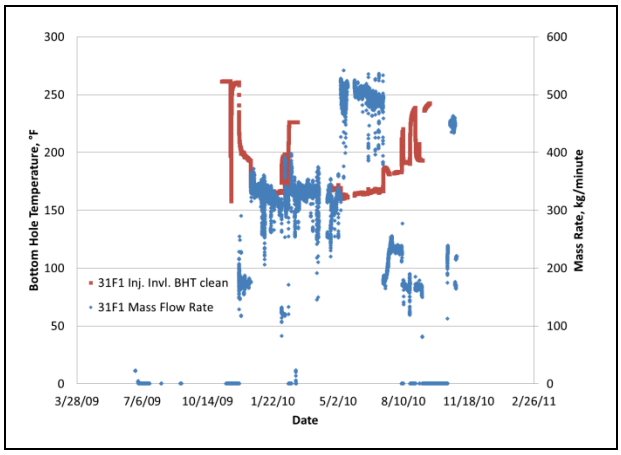

Figure 2. Observed injection rate and bottom-hole temperature at injection well F-1

LBNL Model

Modeling Software

The LBNL Model is based on the numerical simulator TOUGH2 (Pruess et al., 1999) and the equation-of-state module EOS7C (Oldenburg et al., 2004). The EOS7C module is suitable for simulating storage of CO_2 in formations containing water and methane. There is no single TOUGH2 fluid property module presently available that can handle all the features of the S-3 site. EOS7C is used for the present studies, which means that methane can be included but salinity effects on solubility cannot be considered. The temperature range in TOUGH2-EOS7C is wide enough such that the actual formation temperature (~127°C) can be represented.

Model domain and numerical grid

Figure 3 shows the boundaries (thick black lines) of the model domain (4,000 m × 5,200 m) and the numerical grid, which are superimposed on the contour map of the structural dome at the S-3 site. The model covers just one flank of the dome, and for simplicity is modeled as a tilted plane. The plane of the model is tilted two degrees down from the fault (shown in yellow). Voronoi tessellation is used rather than a rectangular grid to allow for local grid refinement and to eliminate grid orientation effects. The red box shows the fine-grid region in which the CO_2 plume is expected to remain. There are 621 gridblocks per layer, and 8 layers, for a total of 4,968 gridblocks.

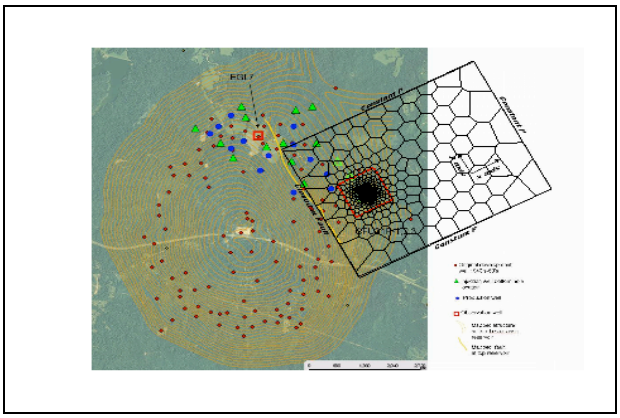

Figure 3. Plan view of the model domain and the numerical grid for the LBNL Model

Rock properties

Permeabilities were inferred from well logs at the injection well (F-1). The first step for assigning model permeabilities was to scale the well-log permeabilities, so that their depth-averaged values over the open interval equaled the permeability values inferred from the well test. Horizontal permeability for the model was obtained by arithmetic averaging of the well-log permeabilities. Vertical permeability was obtained by harmonic averaging of the well-log permeabilities. To reduce vertical permeability relative to horizontal permeability, we also applied an anisotropy factor (0.5).

No lateral property variation in the formation is included. A well test at the injection well indicates a large skin value. This is approximately included in the model by decreasing the permeability in the column of gridblocks representing the injection well, such that the modeled pressure at the injection well matches the observed pressure. No site-specific information is used for characteristic curves. Liquid relative permeability is Corey-like, and gas relative permeability has a similar form. Gas residual saturation is assumed to be zero (i.e., residual-phase trapping is not considered), which is considered reasonable only for the injection period. Capillary pressure strength is inversely proportional to the square root of permeability.

Initial and boundary conditions

Initial conditions for CO_2 injection consist of a water-saturated formation at constant temperature (127°C) and hydrostatic pressure (about 32.0 MPa). The formation water is saturated

with dissolved CH_4. The left boundary of the model is closed to fluid flow, since it coincides with a fault believed to be sealing. The other model boundaries in the horizontal plane (see Figure 3) are constant-pressure boundaries. Top and bottom boundaries are no-flow boundaries.

Injection consists of 92% CO_2 and 8% CH_4 (mole %). A variable injection rate was used in these simulations—see more discussion on this below. Injection was first modeled with a mass source in each model layer corresponding to the open well interval, with the fraction of fluid going into each layer proportional to the permeability-thickness product of that layer. As an alternative, injection was introduced at the top model layer representing the open well interval, with a high vertical permeability assigned to the gridblocks representing the open interval. The second option was finally selected, because it provided more accurate distribution of the CO_2 (i.e., because it accounted for the density difference between water and CO_2).

PNNL MODEL

Modeling software

The PNNL Model is based on the STOMP-WCSE simulator (White and Oostrom, 2006), which can model nonisothermal systems consisting of water, CO_2, and salt. However, it does not include CH_4. This is in contrast to the LBNL Model, which includes CH_4 but ignores the presence of salt.

Model domain and numerical grid

The PNNL Model covers an area of 3,200 m × 3,200 m in the horizontal plane centered on the injection well (F-1), and has 16 layers in the vertical direction. The model domain is bounded on the left-hand side by the sealing fault. A boundary-fitted grid was developed using the surface provided for the top of the lower Tuscaloosa formation. Irregular grid spacing was used to better capture the breakthrough times at the observation wells. There are in total 53×53×16 gridblocks in the numerical grid (Figure 4).

Rock properties

Porosity and permeability values used in the PNNL Model are based on cores obtained from the two observation wells (F-2 and F-3). The measured porosity values have a range of 1.29–31.44% with a mean of 21.76%. Measured permeability values were spread over almost five orders of magnitude (0.01–1890 mD), with a geometric mean of 2.91 mD. From the well logs, a total of 14 facies were identified. For simplicity, these were recombined into three facies: Facies 1 (consisting of sandstone), with porosity of 27% and mean permeability of 360 mD; Facies 2 (consisting of sandstone and limestone), with porosity of 26% and mean permeability of 44 mD; and Facies 3 (all other materials), with porosity of 16% and mean permeability of 9 mD.

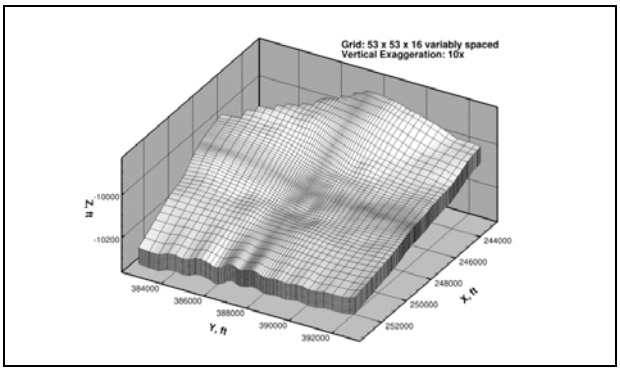

Figure 4. Numerical grid used in the PNNL Model

The program TPROGS (Carle and Fogg, 1997) was used to generate three transition probability-based facies models assuming a fluvial depositional environment. Permeability and porosity were assumed constant within each facies, and different values were assigned to each facies corresponding to the mean values mentioned above. Three additional realizations were generated, where porosity and permeability within each facies followed a uniform random distribution. Finally, three more realizations were generated where porosity and permeability followed a Gaussian random distribution. Overall, nine realizations of the porosity-permeability field were generated.

The thermal properties of the formation were taken from typical values for sand, with a thermal conductivity of 0.582 W/m K and a specific heat capacity of 700 J/kg K. A Brooks-Corey saturation function was fitted to laboratory measurements, using parameters scaling with intrinsic permeability, with an assumed residual saturation of 1%. A Burdine porosity distribu-

tion model was assumed for the calculation of relative permeability. The maximum entrapped gas saturation was assumed to be 20%.

Initial and boundary conditions

The model domain was assigned an initial pressure of 32.3 MPa, a temperature of 128°C, and a dissolved salt mass fraction of 0.157. The initial pressure and temperature were taken from the observed pre-injection values in the injection well. The dissolved salt mass fraction was calculated from the geochemical analysis provided for Lower Tuscaloosa brine. Fluid pressures were allowed to reach hydrostatic equilibrium before the start of CO_2 injection. The four lateral boundaries were held at their initial hydrostatic values, while the corner boundary corresponding to the fault was assumed no-flow. Top and bottom boundaries were also assumed closed to flow.

A well model in STOMP-WCSE was used to simulate CO_2 injection. A well model is defined as a type of source term that extends over multiple grid cells, where the well diameter is smaller than the grid cell. The CO_2 injection rate is proportional to the pressure gradient between the well and the surrounding formation in each grid cell. A bottomhole pressure is calculated iteratively until either maximum borehole pressure or the desired injection rate is reached.

ICL Model

The ICL Model of the S-3 site is based on the E300 module of the ECLIPSE compositional reservoir simulator (http://www.slb.com/services/software/reseng/compositional.aspx). In the E300 module the CO2STORE option was used. This option can handle three phases, which are a CO_2-rich phase, an H_2O-rich phase, and a solid phase. The CO_2-rich phase is labelled the gas phase, while the H_2O-rich phase is labelled the water phase (liquid phase). The mutual solubilities of CO_2 and H_2O are calculated to match experimental data for CO_2-H_2O systems under typical CO_2 storage conditions: 12–100°C and up to 600 bar.

The ICL Model spans a distance of 2000 ft in both the *x* and *y* directions. In the vertical (*z*) direction, the grid is 80 ft thick and centered on the injection well (F-1). Figure 5 shows a schematic diagram of the model domain. Different values of pore volume multipliers were used on each of the four sides of the model to represent the larger size of the site. The grid has 8 layers in the vertical direction. Gridblocks within each layer have the same porosity and permeability values, though they are different from one layer to another. Porosity and permeability values are estimated from core plugs. It is assumed that only water and CO_2 are present in the system. The ICL model uses the actual observed injection rate (Figure 2).

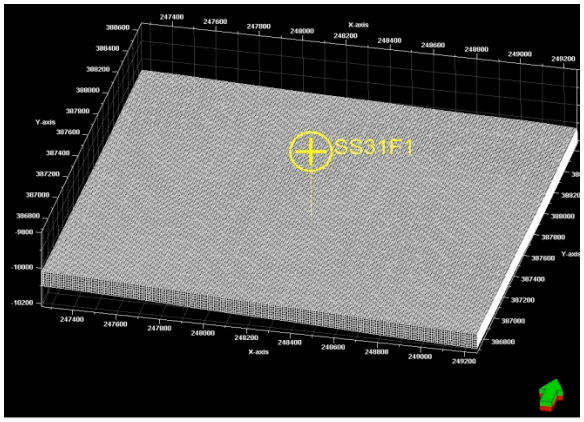

Figure 5. Numerical grid used in the simulations using the ICL Model

VESA Model

The VESA approach (Gasda et al., 2009) is derived through vertical integration of the three-dimensional governing equations for two-phase flow under the assumptions of vertical equilibrium, complete gravity segregation, and capillary equilibrium between CO_2 and brine (Gasda et al., 2009). The resulting model is a two-dimensional model for flow in the lateral directions. The vertically upscaled equations account for fluid and matrix compressibility, as well as hysteresis in the relative permeability function. Solubility of CO_2 in brine is also considered in the upscaled model, which is comprised of equilibrium partitioning into the regions containing residual brine and residual CO_2. No convective mixing is considered in these simulations.

The two-dimensional upscaled equations were discretized on a 201×201 grid using a standard finite difference approximation. The grid has a constant spacing of about 10 ft. For this system,

fluid properties are assumed to be incompressible and constant in space and time. Brooks-Corey-type relative permeability functions are used. The capillary pressure-saturation relation is assumed to be a van Genuchten type. Rock properties are assumed to be homogeneous and isotropic. CO_2 was injected at a constant rate of 4.6 kg/s for a period of 1 year.

RESULTS

Modelers have built their models based on their own interpretation of the site-characterization data provided to them. Caution thus needs to be exercised when comparing the results from one model to another. Note also that the results presented here are obtained through predictive simulations, i.e., the model results are not calibrated to any observation data from the S-3 site except the pressures in the injection well.

LBNL Model

Figure 6 shows the simulated evolution of pressure and gas saturation in the injection (F-1) and two observation wells (F-2 and F-3). It also shows the observed pressure (symbols) at F-1. The predicted pressure at F-1 captures the observed trends in pressure buildup. Note that these predictive simulations were performed using a skin factor of 200. Reducing the skin factor (say, to 100) resulted in a smaller buildup of pressure at F-1. However, changing the skin factor did not have any impact on either the pressure or the saturation response away from the injection well.

Figure 7 shows contours of gas saturation in the layer with the largest permeability at end of injection (1 year). Note that the plume moves only about a few hundred meters away from the injection well at the end of injection. Note also that the plume is mostly radial, with a small preferential movement in the up-dip direction. According to this model, at end of injection (1 year), ~79% of the injected CO_2 remains in the gas phase and the rest is dissolved in water.

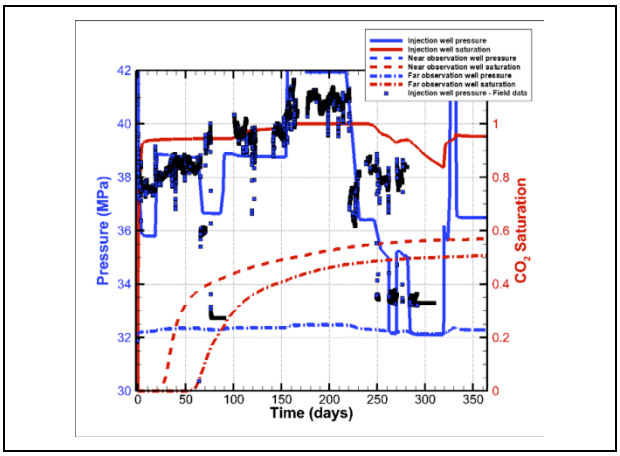

Figure 6. Observed pressure at F-1, and predicted pressure and gas saturation at F-1, F-2, and F-3 using the LBNL Model

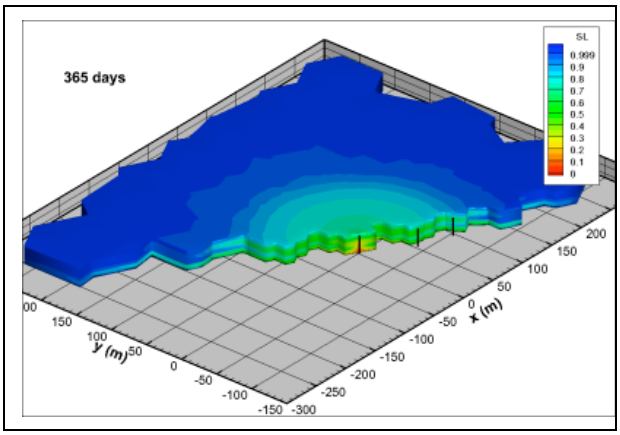

Figure 7. Contours of gas saturation at end of injection. Up-dip direction is towards the right side of the figure

PNNL Model

Analysis of the simulated plume extent using different realizations of the permeability and porosity distributions show that facies orientation, and the distribution of hydraulic properties within each facies, has a significant effect on predictions of supercritical CO_2 saturation and pressure distribution in the formation. As examples, simulated contours of gas-phase saturation at 1 year for Realization #5 (where the property distribution within each facies is uniformly random) and Realization #8 (where the property values within each facies follow a normal distribution) are shown in Figures 8a and 8b, respectively. Preliminary results suggest that realizations with uniform random hydraulic property distribution within each facies match the pressure response at F-1 most closely. The PNNL

Model predicts that about 84% of the injected CO_2 will remain in gas-phase and 16% will undergo dissolution at end of injection.

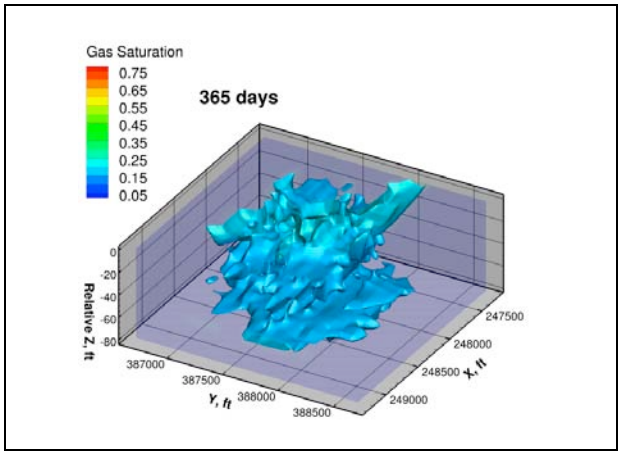

Figure 8a. Contours of CO_2 saturation at 1 year with Realization #5 of the PNNL Model

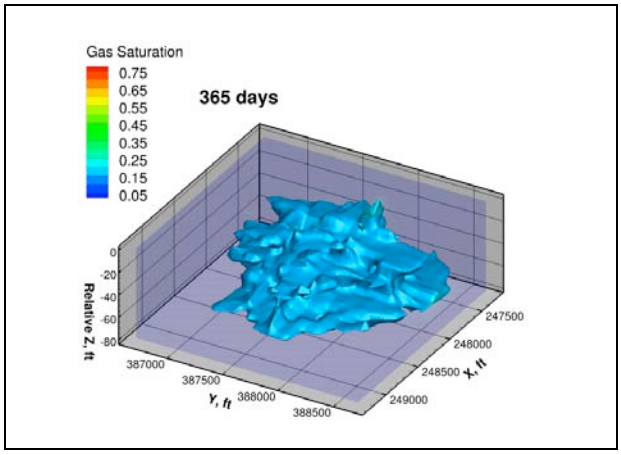

Figure 8b. Contours of CO_2 saturation at 1 year with Realization #8 of the PNNL Model

ICL Model

Simulated contours of the CO_2 saturation at the end of injection (1 year) are shown in Figure 9. The ICL Model predicts that about 86% of the injected CO_2 remains in the gas phase, which is about the same as predicted by the PNNL Model.

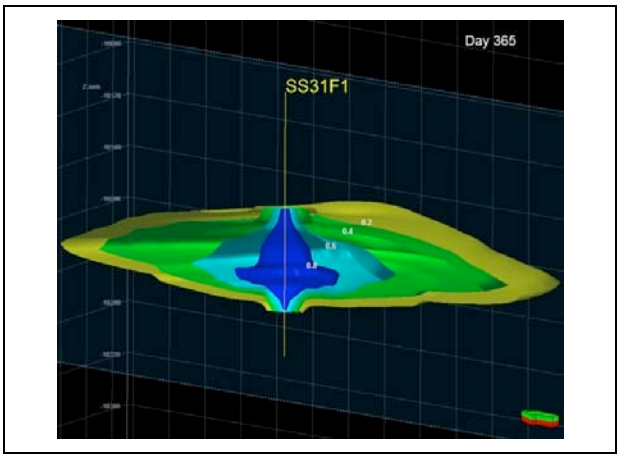

Figure 9. CO_2 contours at 1 year (ICL Model)

VESA Model

Figure 10 shows contours of integrated CO_2 plume thickness at 1 year. In this model, at end of injection, ~95% of the injected CO_2 stays in the gas phase and the rest in brine phase The VESA Model predicts arrival times of 27 days at F-2 and 65 days at F-3.

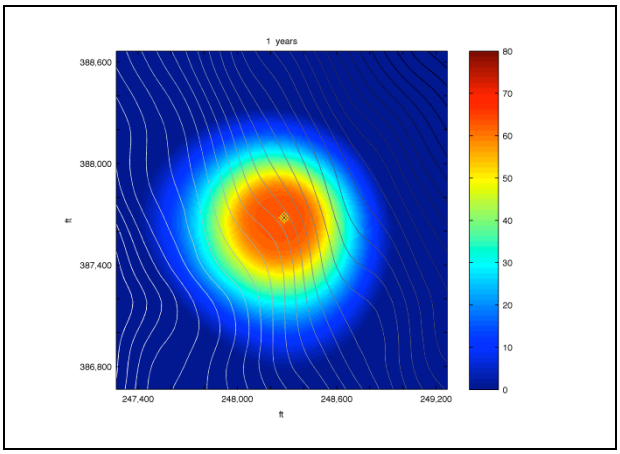

Figure 10. Contours of integrated CO_2 plume thickness in feet at 1 year (VESA Model)

QUALITATIVE MODEL COMPARISON

Even with only four conceptual models, it is clear that model conceptualization varies widely. The differences in conceptualization are reflected in the predictions from these four models. For example, the LBNL Model predicts that CO_2 breakthrough occurs at 19 and 53 days at F-2 and F-3, respectively. Over the nine realizations simulated by the PNNL Model, breakthrough times at F-2 ranged from 8 to 14 days, whereas the same for F-3 was 19 to 53 days (realizations with uniform random property

distribution predict longer breakthrough times). The ICL Model predicts CO_2 arrival times of 36 and 94 days, and the VESA Model predicts breakthrough at 27 and 65 days at wells F-2 and F-3, respectively. If we bracket the range of breakthrough predictions, we have between 8 and 36 days for F-2 and between 19 and 94 days for F-3. This gives an indication of the possible range of uncertainty caused by conceptual model choices, even for a simplified GCS injection scenario. The challenge for modelers is to attempt to reduce this range of uncertainty.

Similarly, if we bracket the fraction of CO_2 in the gas phase after injection ends, we get a minimum of 79% (LBNL) and a maximum of 95% (VESA). One possible reason for this large spread can be how the relative permeability and capillary pressure curves are implemented in each model. For example, the TOUGH2 simulations were performed with nonhysteric characteristic functions and without including residual-phase trapping, resulting in a more spread-out plume, which might have led to more dissolution (and less gas-phase saturation) than would be expected. Clearly, differences in conceptual model choices and numerical implementation cause significant differences in model predictions.

SUMMARY AND CONCLUSIONS

In this paper, we present preliminary predictions made by the TOUGH2 simulator while simulating the CO_2 injection scenario at the S-3 site, whose complex geology poses significant challenges for modelers. These TOUGH2 predictions are compared with those using STOMP, Eclipse, and VESA approaches. From a preliminary comparison of the four models, it is clear that differences in model conceptualization result in a large range of predictions. For example, if we bracket the predicted time for CO_2 arrival at the two observation wells, we have a range of 8–36 days for Well F-2, and 19–94 days at Well F-3. Further, predicted gas-phase saturation at the end of the injection period varies from 79–95%.

The range of prediction uncertainties, of course, will decrease when the models are calibrated to observed data from the S-3 site. Model predictions can be further improved by using more site-specific data, such as the characteristics curves, and by incorporating spatial heterogeneities in key reservoir properties.

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